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Title: IS&T Computing Overview

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Intended for: ALD presentation to Chris Fall and Cathy Tripodi visit to LANL

3/21-22/19; institutional host Mason, technical host Sarrao, organized

out of DDSTE/Protocol planner Peggy Vigil

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IS&T Computing Overview

Emphasis: HPC, QIS, AI/ML

Irene Qualters

ALD, Simulation and Computation

ASCR POC

ECP LOTF

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ALD, Physical Sciences

BES, FES, HEP, NP POC

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DDD, Computational and Statistical Sciences

LANL CRLC member

March 21, 2019





Agenda

March 21, 2019

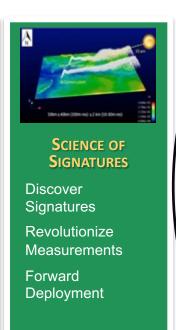
TA-3, Bldg. 123. T Conference Room 218-220

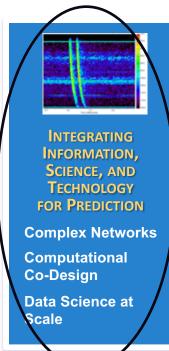


- Introduction to IS&T at LANL
 - Integrated Information Science & Technology (IS&T)as a Core LANL Capability
 - IS&T within the Lab Agenda
 - Office of Science Investments in Simulation and Computation Directorate
- HPC: Exascale and beyond
- Quantum Information Science
- Artificial Intelligence/Machine Learning

Integrating IS&T for Prediction is one of four core capabilities that guide strategic investment to realize LANL mission and vision







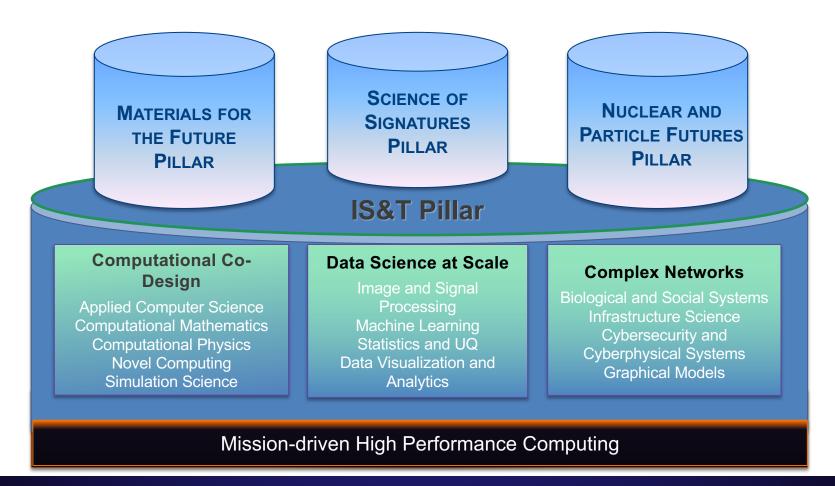


Mission: To solve national security challenges through scientific excellence

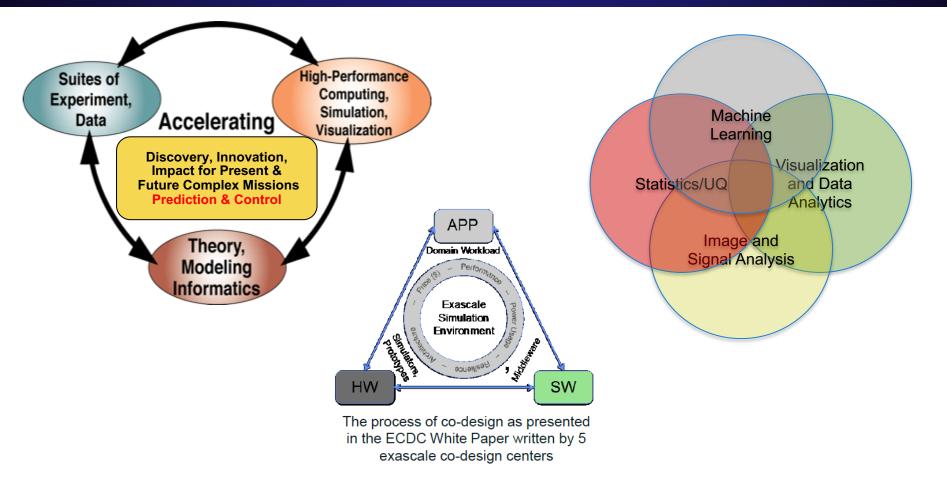
Vision: To deliver science and technology to protect our nation and promote world

stability

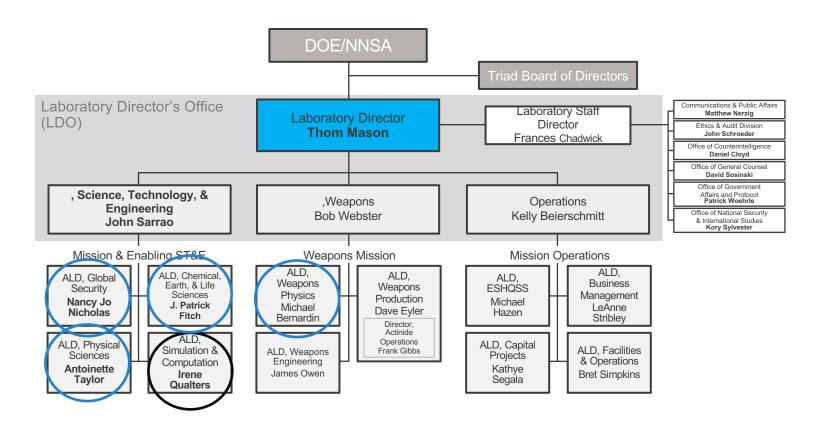
Integrating IS&T for Prediction is a cross-cutting pillar



LANL Approach to IS&T is rooted in CoDesign: Integrated, cross-disciplinary, mission-driven, encompassing evolution and revolution



IS&T Pillar leadership is strongly positioned for cross-cutting effectiveness in the Triad LANL structure



Directorate for Simulation and Computation is home to IS&T Pillar Leadership

Fundamental domain expertise (T-Division) uniquely positions LANL IS&T for multi-disciplinary approaches to technology strategy





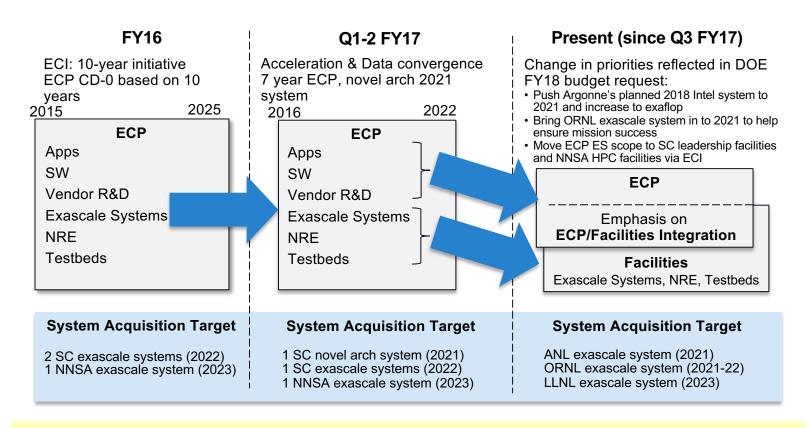




Vibrant and cohesive IS&T capabilities are key to achieving lab agenda

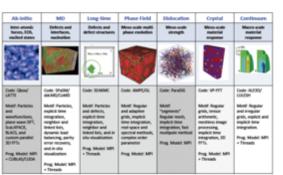
SIMULTANEOUS EXCELLENCE	I. NUCLEAR SECURITY	II. MISSION-FOCUSED SCIENCE, Technology, and Engineering	III. MISSION OPERATIONS	IV. COMMUNITY RELATIONS
Strategic Objective (10–20 years)	Excellence in Nuclear Security	Excellence in Mission-Focused Science, Technology, and Engineering	Excellence in Mission Operations	Excellence in Community Relations
Critical Outcomes (5–10 years)	Design, produce, and certify current and future nuclear weapons and reduce the global nuclear threats	Deliver scientific discovery and technical breakthroughs that support DOE and NNSA missions	Execute sustained operations that are reliable and responsive to mission needs	Sustain and enhance LANL's partnership with the community across the Northern New Mexico (NNM) Region
Major Strategic Initiatives (1–5 years)	I.1. Execute LANL's Manufacturing mission to deliver 30 plutonium pits per year I.2. Transform nuclear weapons warhead design and production I.3. Anucipate threats to global security develop and deploy revolutionary tools to detect, dater, and respond I.4 Achieve First Production Unit (FPU) and Last Production Unit (LPU) for the W88 ALT 370, B61-12 LEP, and ALT 940	ECSE->DMMSC and related capabilities	Ill.1. Achieve culture change with an emphasis on organizational learning III.2. Improve integrated planning across priority mission activities and infrastructure III.3. Address-critical issues related to NMC&A, nuclear safety, criticality safety, and waste III.4. Implement systematic process improvement to drive increased rigor and efficiency in work execution III.5. Enhance quality of work life, workforce planning, and training and development	IV.1. Institute a personal commitment to community service by LANL leadership W.2. Engage in mission-centered workforce and pipeline development IV.3. Enhance small business participation in executing LANL scope across all directions IV.4. Implement a Community Commitment Plan to provide educational, economic development, and philanthropic support to the surrounding community

ECP History: From the Start of Project to Present

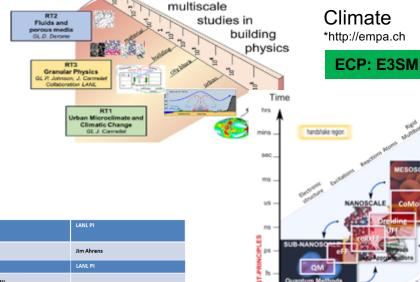


ECP matured, not without local challenges; project end is approaching

LANL is strongly represented across the breadth of ECP governance, applications, and software technologies and also strongly represented in the SCIDAC portfolio



ECP: COPA ExaAM Materials
*Ex Mat Ex



Laboratory of

Lead PI RAPIDS: A SciDAC Institute for Computer Science and Data Rob Ross (ANL) Coupling Approaches for Next-Generation Architectures (CANGA) Philip Jones, LANL Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models Stephen Price, LANL Non-Hydrostatic Dynamics with Multi-Moment Characteristic Discontinuous Galerkin Peter Bosler, SNL Balu Nadiga Methods A New Discrete Element Sea-ice Model for Earth System Modeling Adrian Turner, LANL Nuclear Computational Low Energy Initiative (NUCLEI) Computing the Properties of Matter with Leadership Computing Resources Robert Edwards, TJNAF Boram Yoon William (Raph) Hix, ORNL Chris Fryer Towards Exascale Astrophysics of Mergers and Supernovae (TEAMS) Anders (David) Andersson, LANL Simulation of Fission Gas in Uranium Oxide Nuclear Fuel Accelerating HEP Science: Inference and Machine Learning at Extreme Scales Salman Habib, ANL Earl Lawrence **Tokamak Disruption Simulation** Xianzhu Tang, LANL

Biology
*http://wag.caltech.edu

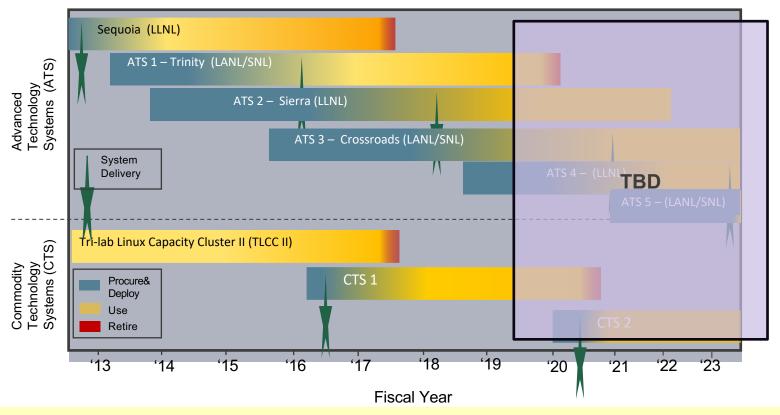
Andres Jaramillo-Botero and William A. Goddard III © 2006

ECP: ExaBiome

Inverse and Direct solutions

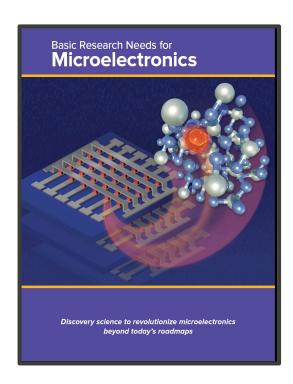
Length

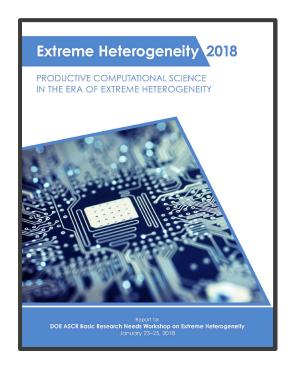
NNSA/ASC is currently revising its platform strategy to account for technological and budgetary realities

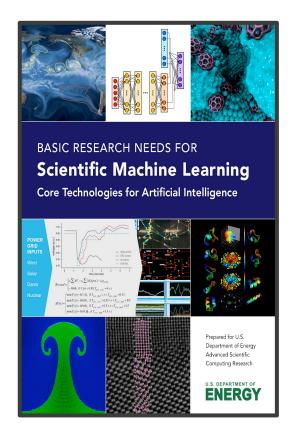


Crossroads proposals due April 8, 2019

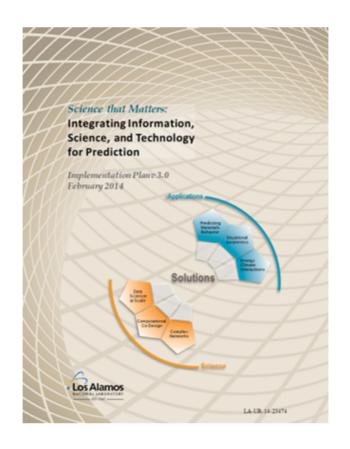
Office of Science Strategic Workshops and Reports are re-examining new opportunities for HPC advances in a diverse, disruptive, and dynamic technology landscape

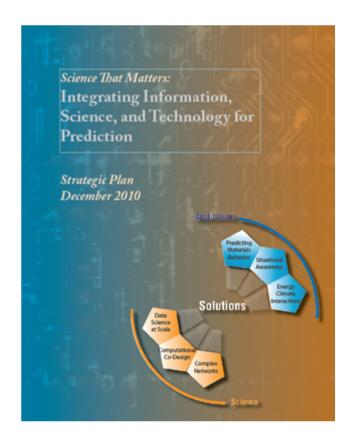






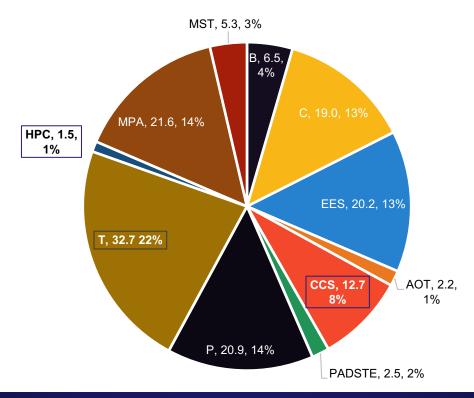
IS&T Strategy Refresh planned: integrating ASC, ASCR priorities





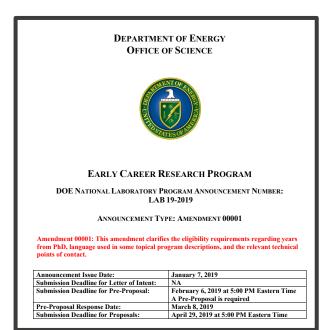
DOE SC Investment in Simulation and Computation Divisions spans HEP, NP, BER, BES, ASCR programs

DOE-Office of Science FY18 Confirmed Budget by LANL
Division (\$M) Including Previous Year Carryover
(Total = \$151M)

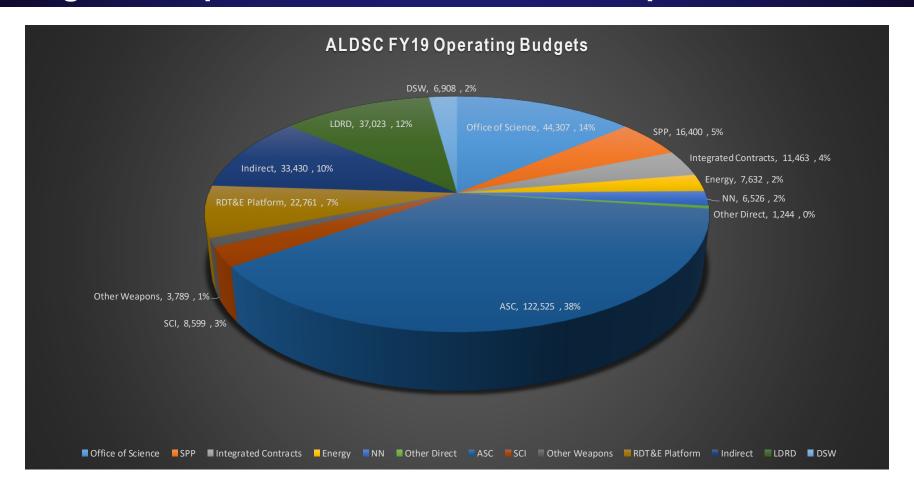


FY19 Early Career Awards have strong LANL participation

- LANL submitted 25 Pre-proposals (there were 22 last year)
 - ASCR-3; BER-5; BES-12; FES-3; HEP-1; NP-1
- Applicants were from 10 LANL Divisions
 - A-1; AOT-1; B-1; C-3; CCS-1; EES-4; MPA-5; MST-2; P-3; T-4
 - ASCR: CCS-7; Irina Demeshko; "A Framework for Highly Parallel Task-based, Asynchronous Multilevel Solvers"
 - ASCR:T-5; Guangye Chen; "Unsupervised-learning-assisted Multiscale Algorithms for Kinetic Systems of Arbitrary Collisionality"
 - BES: T-1; Enrique Martinez Saez; "Integrated Mechano-Chemical Framework to Understand the Radiation Response of Multicomponent Concentrated Alloys"
 - BES: T-4; Shi-Zeng Lin; "Theoretical Study of Novel Quantum States Stabilized by Magnetic Spin Textures"
 - NP: T-2; Emanuele Mereghetti; "Nuclear effective theories for searches of physics beyond the Standard Model"



2019 Office of Science research investments are a significant portion of the SC directorate portfolio



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LANL has been involved in QIS Since the Beginning



Illustration from Wojciech Zurek's "Decoherence and the Transition from Quantum to Classical", *Physics Today* (1991).

Zurek (still at LANL) is known for foundations of quantum decoherence, the Kibble-Zurek mechanism, and the no-cloning theorem.



Quantum Lunch seminar series

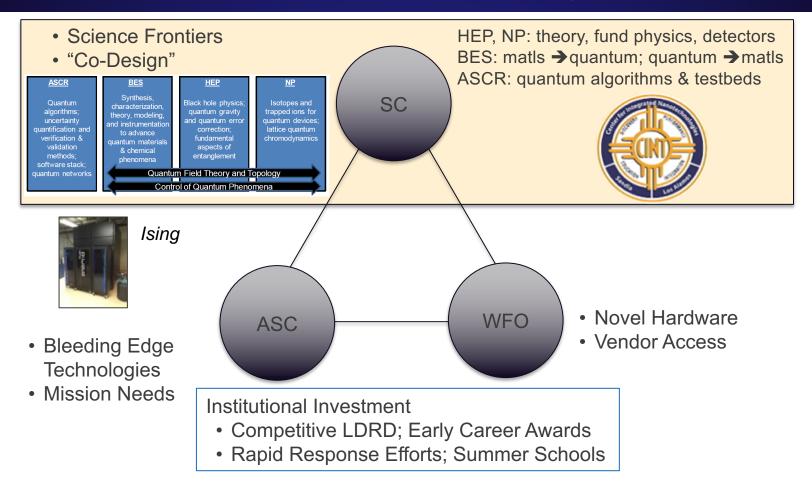
- http://quantum.lanl.gov/qlunch/
- One talk every 1–2 weeks, running uninterrupted since 1992
- Both internal speakers and visitors to the Laboratory, from postdocs to luminaries in the field
- Broad coverage of QIS-related topics

LANL's current approach to QIS is consistent with the goals of the Lab Agenda

- "Breadth over depth"
 - Cover as many aspects of quantum computing as possible
 - Don't know a priori what will turn out to be useful so try everything
- Consider both gate-model quantum computing and quantum annealing
- Develop partnership strategies: Compete or collaborate?
- Invest internal funds into different types of investigations
 - Fundamental science, with internal investments from the Laboratory Directed Research and Development office
 - Additional funding through competitive proposals from DOE Office of Science (ASCR, BES, HEP)
 - Delivery of Mission needs: investments from the Advanced Simulation and Computing program
- Additional emphasis on education
 - Internal funding through the National Security Education Center
 - Train the LANL workforce—in particular, staff members with no background in anything quantum-related—to program quantum computers
 - Train students in quantum information processing and hope they one day become LANL staff

- Address research challenges crosscutting physics, computing, & materials

LANL has a multi-faceted Quantum Strategy that connects fundamental R&D with our NNSA and broader national security missions.



Office of Science investments enable foundational R&D in QIS at LANL



Advanced Scientific Computing Research

- Optimization, Verification and Engineered Reliability of Quantum Computers, (SNL led)
- Quantum Algorithms from the Interplay of Simulation, Optimization, and Machine Learning (SNL led)

Basic Energy Sciences

- Topological phases of quantum matter and decoherence
- Deterministic placement and integration of quantum defects, (CINT, LANL)
- Quantum Sensed Nuclear Magnetic Resonance Discovery Platform, (CINT, SNL)

High Energy Physics

- Quantum Computing for Quantum Field Theories and Chiral Fermions
- Quantum Computing for Neutrino Nucleus Dynamics
- Quantum Foundations on Quantum Computers
- Quantum Machine Learning Enhancing Lattice QCD Calculations of Matrix Elements for Beyond the Standard Model Physics Search New proposal calls in QIS underway from BES and HEP.
 QIS calls from Nuclear Physics and Fusion Energy Science are forthcoming.

The Center for Integrated Technologies (CINT) is leading the DOE-BES Nanocenters in nano→QIS S&T.



New Quantum Materials Thrust with a focus on understanding and controlling quantum effects in nanoscale materials and their integration into systems spanning multiple length scales.

- Capabilities to fabricate Qubits and next generation nanomaterials
 - Fabrication of donor-dot (and other structures) qubit devices in semiconductor systems
 - Next generation QIS materials e.g. single photon sources, topological materials
- Capabilities to characterize Qubits and next gen QIS materials
 - Single spin characterization and single photon measurements at high magnetic fields
 - State of the art instrumentation to study single nanostructures and single photons, including optical spectroscopy systems equipped with a 9T magnet
- Strong Theory support coupled to QIS effort at host labs
 - Real-time density functional theory, time-dependent Lanczos and dynamical mean-field theoretical methods, to tackle both weakly and strongly correlated quantum materials

Three areas identified in CINT strategic plan for expansion:

- 1. Deterministic placement and electronic/photonic integration of solitary quantum defects.
- 2. Build Quantum-sensed Nuclear Magnetic Resonance (NMR) Discovery PlatformTM.
- 3. Using light to probe and control novel phenomena in quantum materials.

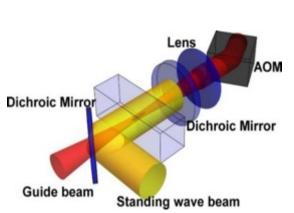
Our QIS portfolio supports development of quantum sensors to improve inertial navigation for DOD missions.



Atomic-Photonic Integration (A-Phl) Program:

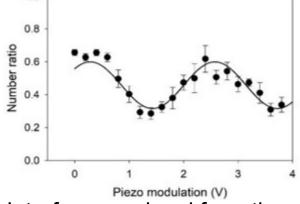
"The A-PhI program will develop trapped-atom based, high performance Position, Navigation and Timing devices and reduce the complexity of these atomic systems using Photonic Integrated Circuits.A-PhI will also demonstrate proof-of-concept trapped atom gyroscopes, a matter-wave analogue of the interferometric fiberoptic gyroscope" (Program motivated in part by LANL's matter wave circuitry technology developed by LDRD.)

LANL has developed the world's first waveguide Sagnac atom interferometer



Los Alamos National Laboratory

Goal: Realize a Sagnac atom interferometer using a moving atomic waveguide to contain a BEC that is split, reflected and recombined. The motion of the waveguide means that the interferometer encloses an area.



Interference signal from the Sagnac atom interferometer.

We are applying quantum communications & cryptography techniques to improve the security of the electric grid

Objective

Use quantum key distribution (QKD) to secure control systems data with acceptable latency

 Existing crypto cannot authenticate within latency requirement

Result

Fully operational with existing SCADA hardware

Multicast authentication within latency requirement

> Industry-standard phasor data concentrator

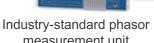


PI: Ray Newell

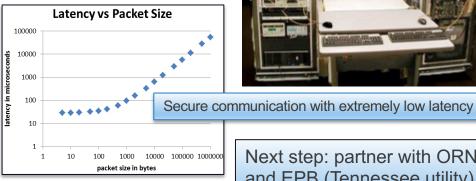
Sponsor:: Office of Cybersecurity, Energy Security, and Emergency Response (CESER)







measurement unit



Next step: partner with ORNL and EPB (Tennessee utility) to demonstrate metro-scale QKD.

75 km

Los Alamos National Laboratory

LANL acquired a D-wave quantum annealer supported by NNSA's Advanced Simulation and Computing Program

- D-Wave quantum annealer 2X "Ising", ~1000 qubits
- Shared resource usage model on open network
 - Focus is to develop collaborative network of people and ideas
 - External users/collaborators welcome
 - Makes LANL the world's first "quantum user facility"

Reaping benefits of local access

- Unmetered access encourages experimentation and enables QC community growth
- D-Wave staff member on-site at LANL since 2016 giving technical advice & assistance and providing on-site D-Wave tutorials spanning multiple levels of expertise.
- LANL has developed multiple open-source software packages for the D-Wave
- Usage stats (Nov 2016–May 2018): Jobs executed: 291,847,888 (9,629 QPU hours), Average utilization: 70%
- Leading to emerging collaborations with other quantum computing vendors
 - Rigetti, Intel, IBM



LANL's outreach and community engagement is through the National Security Education Center (NSEC) and other venues

International Workshops (Center for Nonlinear Studies)

Quantum Computing and Information for Nuclear Physics

Drury Plaza Hotel, Santa Fe, NM January 23-25, 2019

 The Institute for Materials Science (IMS) is sponsoring a Quantum Matter Visitors Group in the summer of 2019, with Joel Moore, Allan MacDonald, and Todari Senthil forming the inaugural members for 2019.



- LANL IMS and ISTI leads participating on organizing committee for UC/ Lab QIS Workshop
- LANL (Candy Culhane) co-leading the 2019 IEEE Quantum Initiative.

In concert with the directions articulated in the National Quantum Initiative, LANL is exploring complementary alliances and partnerships

- Regionally centered partnership—draws coordinates complementary resources "under one roof" in the Rio Grande Corridor:
 - LANL, Sandia; UNM; University of Colorado; Boulder; regional industries
 - Fundamental research (including industry-funded) and workforce development
 - Higher TRL R&D, IP-protected CRADA's and national security connection at LANL & Sandia
 - QIS Industry Engagement
 - Coordination with NIST
- Quantum S&T Thrusts: Quantum Computing and Simulation; Quantum Networks and Communications; Quantum Matter and Dynamics; Quantum Sensing and Metrology
- Leverages: DOE User Facilities (e.g., CINT); DOE & industry QC testbeds; HPC
- Builds on LANL's strengths in quantum and quant-information theory, many-body physics, device physics, quantum sensors, HPC, q-simulation & annealing, quantum computation and algorithms, materials co-design
- Additional partnership formed with LLNL and PNNL for WFO national security sponsors.

Final thoughts/summary

- LANL has a long history with all things quantum
 - Quantum computing, quantum sensing, quantum information, quantum materials
- We are pursuing a multi-faceted Quantum Strategy that connects fundamental R&D with our NNSA and broader national security missions.
 - Target precious internal funds towards groundbreaking quantum-related research
 - Vigorously pursue competitive opportunities in Office of Science and other sponsors
- Bold move: procurement of a D-Wave quantum annealer
 - Can we identify its strengths and learn how to take advantage of them?
- Unique aspect of LANL's approach: education in QC of non-experts
 - Grow a community of QC users from spanning science disciplines
 - Establish a pipeline of QC users and researchers into the Lab, with an exciting science base as a key draw
- We are developing partnerships to be ready to exploit QIS funding opportunities.
- QIS is a fiercely competitive arena with staffing challenges that are combined with the need to work the boundaries of open/secure environment.

Agenda

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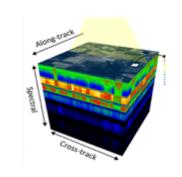
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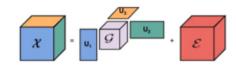


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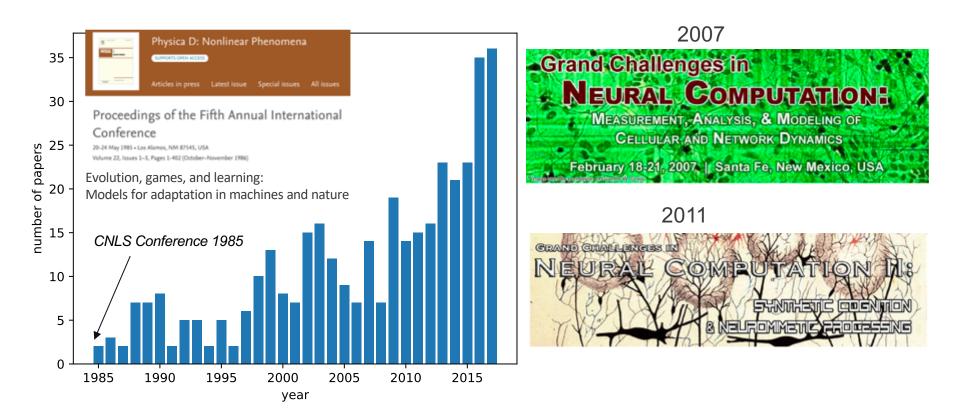
LANL is developing machine learning for science and security missions

- ML has expanded rapidly at LANL
- Converging communities of multidisciplinary researchers
- Leveraging historical strengths in computational physics – "physics-informed ML"
- Investing with LDRD program to develop capability and teams for mission
- Engaging community through workshops and conferences
- Developing pipeline with schools and student internships.





Machine Learning at LANL dates back to 1985



Machine Learning at LANL intersects applications and experts

- Community of >100 researchers spanning from software tool users, through advanced practitioners (~30), to experts (~10).
 Approximately \$15M/year, increasing rapidly.
- Some areas where LANL is developing and applying ML
 - Materials science: Experimental design, molecular dynamics
 - Energy infrastructure: Electrical system parameter learning
 - Theory: Graphical models, sparse coding, reduced order modeling
 - Cybersecurity: Anomaly detection, classification
 - Image and video analytics: Global security
 - **HPC**: Performance prediction
 - Geophysics: Earthquake prediction, low-yield nuclear monitoring
- LANL is on par with National Laboratory peers and benefitting from significant investment in academic and industrial R&D
- LANL focus is on mission science applications

ALDSC Machine Learning Technical Capabilities

· CCS:

- CCS-6: Statistics: Bayesian methods, gaussian process models, emulators
- CCS-3: ML methods: Deep learning, random forest, dictionary learning, computer vision
- CCS-7: Visualization: Large data analysis, in-situ analysis

• T:

- T-1: Chemistry/Materials: ML for MD and Quantum Chemistry
- T-4: Statistical Physics: Graphical Models, Emulators
- T-5: Applied Math: Inverse problems, dictionary learning, sparse coding
- T-6: Biostatistics

HPC

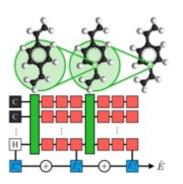
HPC-DES: High-performance computing system analysis

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Applications to Mission Science

NNSA/ASC

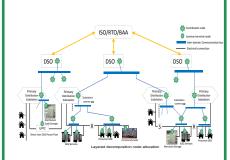
Quantum Chemistry and Molecular Dynamics



Use ML to construct potentials based upon large datasets of quantum calculations

OE/GMLC: AE, A, T

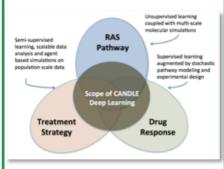
Electric Grid



Graphical models for optimal power flow

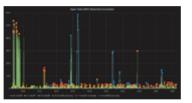
DOE/NCI: B, T, CCS

Cancer



Deep learning for MD, drug response, personalized treatment NNSA/ASC: HPC

High Performance Computing



Detected Anomalies

Process system logs to identify & correct network, storage & application issues.

FY19 new starts in machine learning

LDRD (total \$20M over 3 years)

- Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics
- Enabling Predictive Scale-Bridging Simulations through Active Learning
- Machine Learning for Turbulence
- Taming Defects in Quantum Computers (part ML)
- Statistical Learning in Cyberphysical Systems
- Towards Memristor Supremacy with Novel Machine Learning Algorithms

ASC (\$4M FY19)

- Quantum Aware MD potentials
- Materials modeling in RISTRA
- Nuclear Data Evaluation
- Scheduling jobs on HPC
- Turbulence
- Multiple efforts on Strength/Damage modeling
- Radiograph Analysis

LANL is playing a role in convening and coordinating the machine learning community with workshops and conferences

2019 2018 Machine Learning for January 2018 – Santa **Computational Fluid** Fe and Solid Dynamics 2nd Physics-Informed PHYSICS INFORMED MACHINE LEARNING February 19-21, 2019 Santa Fe, New Mexico Machine Learning SANTA FE. NEW MEXICO SANTA FE. NEW MEXICO MACHINE LEARNING IN SOLID EARTH GEOSCIENCE MACHINE LEARNING IN SOLID EARTH GEOSCIENCE

March 7-9, 2018 | Santa Fe, New Mexico Exploring Data-Focused Research across the Department of Energy

To be continued

- Data and Information Fusion, August 2018
- CoDA 2020

• ..

We are actively developing pipelines through schools and fellowships

Applied Machine Learning Summer Research Fellowship

Los Alamos National Laboratory



2018 2nd Applied Machine Learning Research Internship with larger scope

- 24 Graduate Students (226 applied)
- Working on LANL problems
- Mentors from across LANL applications and organizations

Quantum Neuromorphic Machine Learning

Hierarchical Sparse Coding for Language

Learning Tree Models with Latent Variables

Interpreting Gaussian Graphical Models

When to transfer? Information estimation of feature representation for Transfer

Learning of Convolutional Neural Networks

Molecular Property Modeling Using Machine Learning

Troll Hunter: Understanding Swarm Behavior in Social Networks

Characterization of High Performance Computing Sensor Data

Non-negative Matrix Factorization (NMF) Applied to Molecular Dynamics

Simulations of Protein X-Ray Diffraction

Machine Learning of First-Principle Particle Simulation Data on Particle Acceleration during Magnetic Reconnection

Hyperspectral Detection of Variable and Multiple Targets with Matched Data Pairs

Fast and Efficient Inferning Networks for Graph Partitioning

Learned Structured Sparse Coding with Lateral Inhibition

Efficient Seismic Event Detection using RPCA

Detecting Underground Nuclear Explosion Signatures

Forecasting CO2-driven cold-water geyser eruptions

Machine learning solutions to revealing the hidden seismicity of Mars

Earthquake Similarity through Graphical Modeling of Arrival Time Data

Prediction of Stress Fields with Physics Informed Convolutional Neural Networks
Physics Informed Machine Learning for Backbone Identification in Discrete Fracture

Networks

Detecting Atmospheric Source Locations with Neural Networks

Thank you Questions/Discussion